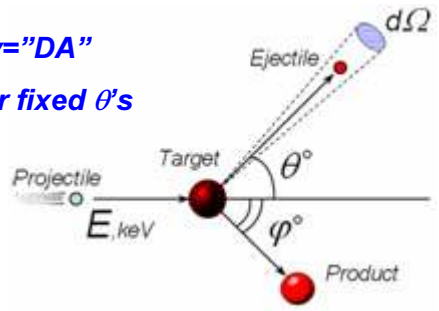
EXFOR to R33 conversion algorithm notes.

V.Zerkin, IAEA-NDS, 13 December, 2007 - 15 January, 2008.

R33 is a format used in Ion Beam Analysis Nuclear Data Library (http://www-nds.iaea.org/ibandl/) for presenting of differential cross sections: dσ/dΩ(E) with fixed angles (θ). Data of similar type are also stored, regularly updated and publicly available for users in EXFOR database. In order to provide a convenient access to the Ion Beam Analysis users community to the EXFOR data and facilitate input of EXFOR data to IBANDL, an automatic conversion procedure is developed in the IAEA-NDS to be used under Web Retrieval System: http://www-nds.iaea.org/exfor/. First version of the conversion was presented on IAEA-CRP meeting in June 2007, where general approach was approved and further improvements were formulated. Beyond simple re-formatting, the conversion procedure uses some assumptions and performs re-calculations. Some details of the used algorithm are described below.

EXFOR: Quantity="DA"

R33: dσ/dΩ(E) for fixed θ's



Content

1. General notes

EXFOR data search program defines whether or not data are appropriate for presentation in R33 format (subsets of data with Quantity=”DA”) and offers launching of conversion procedure.

Conversion of data from EXFOR to R33 is performed for every single EXFOR dataset separately (EXFOR dataset is uniquely identified by Subentry Accession number and Pointer) via intermediate computational format C4.

Conversion to C4 is performed by X4TOC4 program (R.Cullen, A.Trkov) using an artificial dictionary file EXFOR14A.DAT automatically constructed it on the fly. This allows converting almost all relevant EXFOR data to R33 without extension of the dictionary. The system now is able to convert angular distributions of cross sections and Rutherford ratios.

Further operations: display of multi-R33 file for an EXFOR dataset (with sub-sections), selection of R33 file, interactive Web and local plotting.

2. Q-values

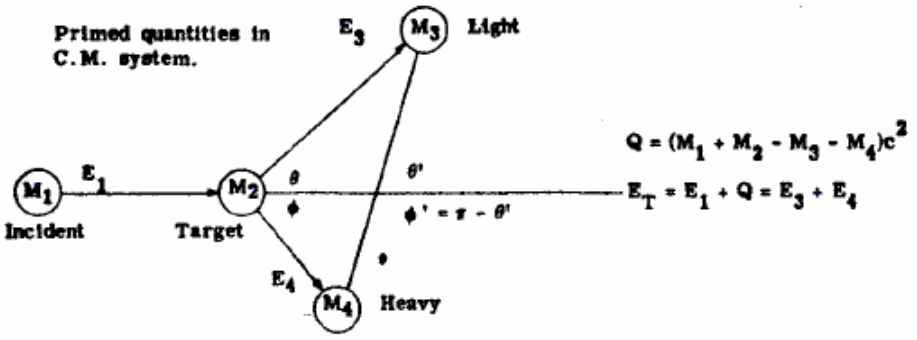
Q-value required in R33 formatted files is not included to EXFOR database. Input data for calculation of Q-value are taken from [1].

3. R33 reaction coding

Coding of reactions in R33 format includes excited state of an outgoing particle. (IBANDL documentation: *“For example, 16O(d,p1)17O is the (d,p) reaction which leaves the residual 17 oxygen in the 1st”*). EXFOR format is using energy level (data with header “E-LVL”) for the same purpose. Conversion procedure uses levels data from RIPL-2 [2].

4. Conversion from C.M. to Lab.

Conversion of data from centre of mass (C.M.) to laboratory system is done using formulas provided by M.Mayer (Fig.1) and A.Gurbich. Cases, where cross sections are given in C.M. but angles in Lab, are marked by the text "**(Angle: not converted)**".



Define:

$$A_{14} = \frac{M_1 M_4 (E_1/E_T)}{(M_1 + M_2)(M_3 + M_4)}, \qquad A_{23} = \frac{M_2 M_3}{(M_1 + M_2)(M_3 + M_4)} \left(1 + \frac{M_1}{M_2}\frac{Q}{E_T}\right) = \frac{E'_4}{E_T}$$

$$A_{13} = \frac{M_1 M_3 (E_1/E_T)}{(M_1 + M_2)(M_3 + M_4)}, \qquad A_{24} = \frac{M_2 M_4}{(M_1 + M_2)(M_3 + M_4)} \left(1 + \frac{M_1}{M_2}\frac{Q}{E_T}\right) = \frac{E'_3}{E_T}$$

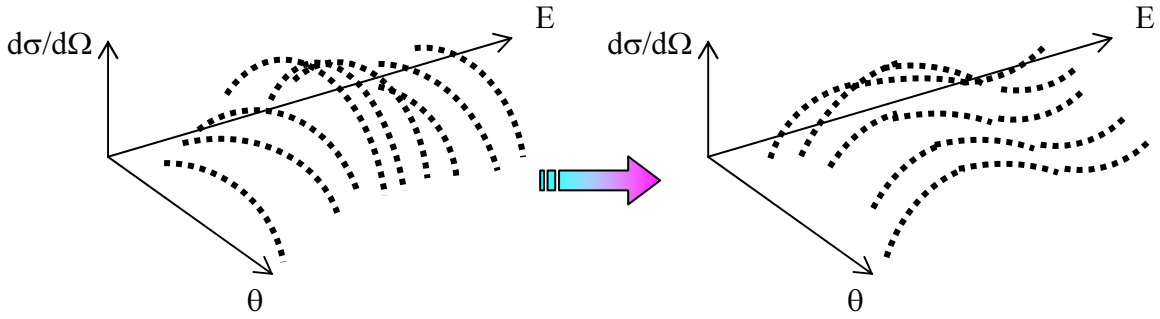
Note that $A_{14} + A_{13} + A_{23} + A_{24} = 1$

Lab energy of light product:	$\frac{E_3}{E_T} = A_{13} + A_{24} + 2(A_{14}A_{23})^{\frac{1}{2}} \cos\theta' = A_{13}\left[\cos\theta \pm (A_{24}/A_{13} - \sin^2\theta)^{\frac{1}{2}}\right]^2$	Use only plus sign unless $A_{13} > A_{24}$, in which case $\theta_{max} = \sin^{-1}(A_{24}/A_{13})^{\frac{1}{2}}$
Lab energy of heavy product:	$\frac{E_4}{E_T} = A_{14} + A_{23} + 2(A_{14}A_{23})^{\frac{1}{2}} \cos\phi' = A_{14}\left[\cos\phi \pm (A_{23}/A_{14} - \sin^2\phi)^{\frac{1}{2}}\right]^2$	Use only plus sign unless $A_{14} > A_{23}$, in which case $\phi_{max} = \sin^{-1}(A_{23}/A_{14})^{\frac{1}{2}}$
Lab angle of heavy product:	$\sin\phi = \left(\frac{M_3 E_3}{M_4 E_4}\right)^{\frac{1}{2}} \sin\theta$	**C.M. angle of light product:** $\sin\theta' = \left(\frac{E_3/E_T}{A_{24}}\right)^{\frac{1}{2}} \sin\theta$
Intensity or solid-angle ratio for light product:	$\frac{\sigma(\theta')}{\sigma(\theta)} = \frac{I(\theta')}{I(\theta)} = \frac{\sin\theta\, d\theta}{\sin\theta'\, d\theta'} = \frac{\sin^2\theta}{\sin^2\theta'} \cos(\theta' - \theta) = \frac{(A_{14}A_{23})^{\frac{1}{2}} (A_{24}/A_{13} - \sin^2\theta)^{\frac{1}{2}}}{E_3/E_T}$	
Intensity or solid-angle ratio for heavy product:	$\frac{\sigma(\phi')}{\sigma(\phi)} = \frac{I(\phi')}{I(\phi)} = \frac{\sin\phi\, d\phi}{\sin\phi'\, d\phi'} = \frac{\sin^2\phi}{\sin^2\phi'} \cos(\phi' - \phi) = \frac{(A_{14}A_{23})^{\frac{1}{2}} (A_{23}/A_{14} - \sin^2\phi)^{\frac{1}{2}}}{E_4/E_T}$	
Intensity or solid-angle ratio for associated particles in the lab system:	$\frac{\sigma(\phi)}{\sigma(\theta)} = \frac{I(\phi)}{I(\theta)} = \frac{\sin\theta\, d\theta}{\sin\phi\, d\phi} = \frac{\sin^2\theta}{\sin^2\phi} \frac{\cos(\theta' - \theta)}{\cos(\phi' - \phi)}$	

Fig.1 Quantities used for the calculation of nuclear reaction kinematics [3].

5. Grouping and averaging.

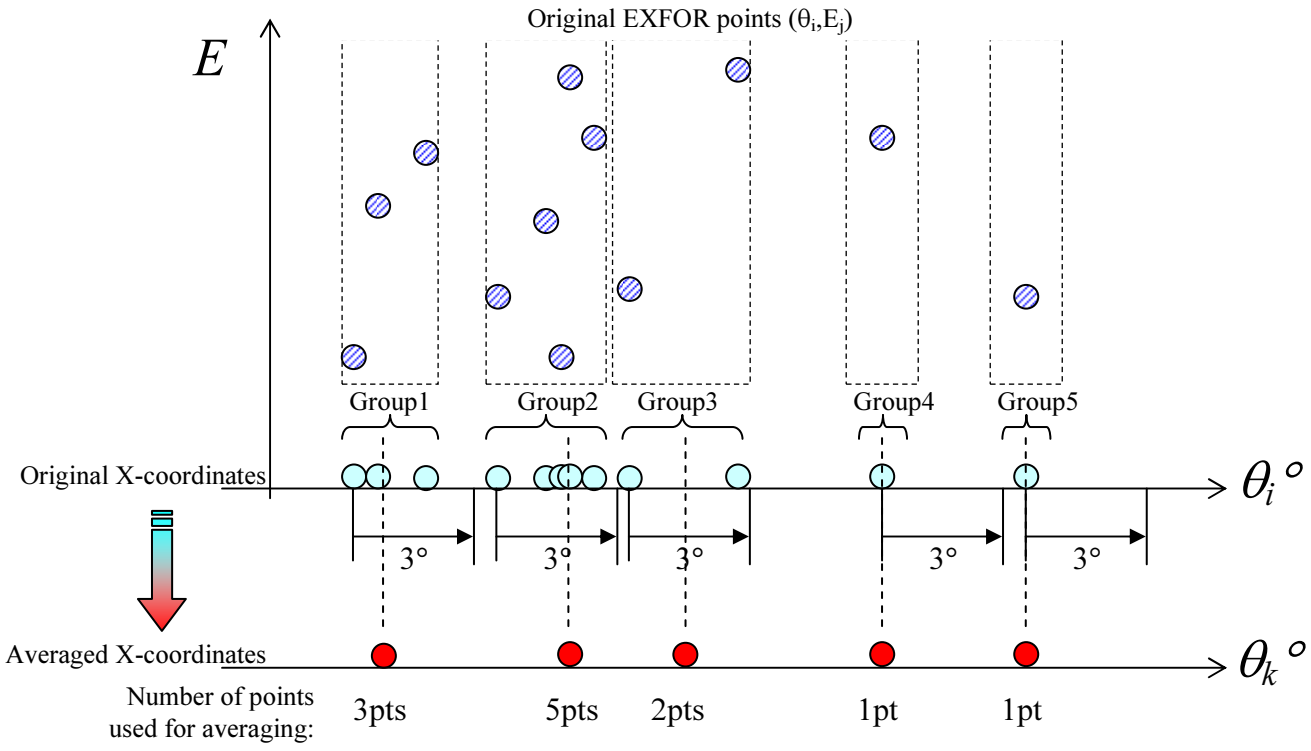
EXFOR allows very flexible data presentation. In cases when data are given as $d\sigma/d\Omega(E,\theta)$ or $d\sigma/d\Omega(\theta)$ for set of E_j some procedures are performed to get data in the form required in R33: set of data $d\sigma/d\Omega(E_j)$. The procedure contains two steps: grouping of angles and averaging of cross sections.



5.a) Grouping of angles.

Input: EXFOR data are given as $d\sigma/d\Omega(E_j,\theta_i)$.
Purpose: to define groups with averaged of angles θ_k.

Default θ averaging interval: $\Delta\theta = 3°$.
a) program finds groups: first points and next few points with $\theta_{next} < \theta_{first} + \Delta\theta$;
b) θ_k is calculated as average of θ's of the group;
c) θ_k is rounded to the nearest 1/10 value;
d) C.M.: cross sections are re-calculated to Lab for new θ_k.



5.b) Averaging of cross sections.

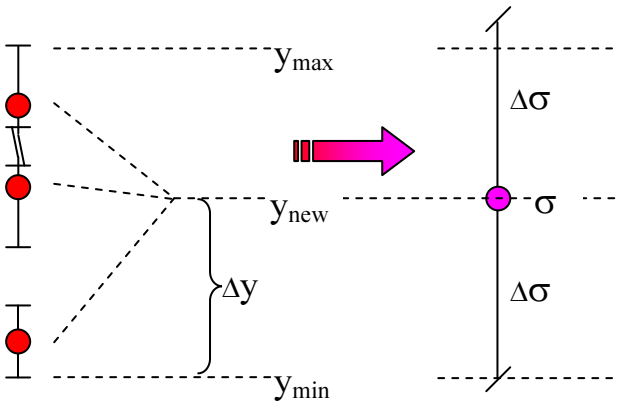
After grouping it may appear that some of the data $d\sigma/d\Omega(E_j)$ have exactly the same energy E_j for several points. For such cases an "Averaging of cross section" is performed:

σ = Average of y_j

$y_{max} = \max \{y_j+\Delta y_j\}$

$y_{min} = \min \{y_j-\Delta y_j\}$

$\Delta\sigma = \max \{ (y_{max} - \sigma), (\sigma - y_{min}) \}$



6. Known problems and possible improvements

1) IBANDL documentation: *"Some cross sections may be sums of several particle groups corresponding to different excited states of the compound or product nucleus. Usually such a cross section would be used when the particle groups are not resolved by the detection method employed. In this case, the postfix lists the states concerned, separated by plus signs. E.g. 14N(d,p5+6)15N."* Not yet implemented, although coded in EXFOR and can appear in C4 file. Suggested by A.Gurbich, December 2007.

2) Data of the same nature the same experimental work can be coded in EXFOR having the same Reaction code but in different Subentries. It would be better to display such data in one EXFOR-R33 session (V.Zerkin, December 2007).

3) Problem: X4TOC4 does not recognize cases where EXFOR present information in two systems simultaneously, like cross section in centre of mass and angle in laboratory system (C4 has only one flag for all combinations CM-Lab). Conversion X4R33 has to treat such cases (V.Zerkin, December 2007). Implemented in January 2008.

4) Conversion for natural elements, e.g. for reaction: *natTi(p,p0)natTi* . (V.Zerkin, January 2008). Implemented 2008-01-15.

5) Your suggestions are welcome……

Bibliography

[1] G.Audi, A.H.Wapstra and C.Thibault, The Ame2003 atomic mass evaluation (II), Nuclear Physics A729 p. 337-676, December 22, 2003, http://www-nds.iaea.org/masses/

[2] T. Belgya, O. Bersillon, R. Capote, T. Fukahori, G. Zhigang, S. Goriely, M. Herman, A.V. Ignatyuk, S. Kailas, A. Koning, P. Oblozinsky, V. Plujko and P. Young, Handbook for calculations of nuclear reaction data, RIPL-2, IAEA-TECDOC-1506, IAEA, Vienna, 2006. http://www-nds.iaea.org/RIPL-2/

[3] N. Jarmie and J.D. Seagrave. Charged particle cross sections. Tech. Rep. LA-2014, Los Alamos Scientific Laboratory, University of California, Los Alamos, New Mexico, U.S.A., 1956.